

# An Efficient Molecular Dynamics Scheme for Predicting Dopant Implant Profiles in Semiconductors

Keith M. Beardmore and Niels Grønbech-Jensen

*Theoretical Division, Los Alamos National Laboratory,  
Los Alamos, NM 87545, USA*

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## Abstract

We present a highly efficient molecular dynamics scheme for calculating the concentration profile of dopants implanted in group-IV alloy, and III-V zinc blende structure materials. Our program incorporates methods for reducing computational overhead, plus a rare event algorithm to give statistical accuracy over several orders of magnitude change in the dopant concentration. The code uses a molecular dynamics (MD) model, instead of the binary collision approximation (BCA) used in implant simulators such as TRIM and Marlowe, to describe ion-target interactions. Atomic interactions are described by a combination of ‘many-body’ and screened Coulomb potentials. Inelastic energy loss is accounted for using a Firsov model, and electronic stopping is described by a Brandt-Kitagawa model which contains the single adjustable parameter for the entire scheme. Thus, the program is easily extensible to new ion-target combinations with the minimum of tuning, and is predictive over a wide range of implant energies and angles. The scheme is especially suited for calculating profiles due to low energy, large angle implants, and for situations where a predictive capability is required with the minimum of experimental validation. We give examples of using our code to calculate concentration profiles and 2D ‘point response’ profiles of dopants in crystalline silicon, silicon-germanium blends, and gallium-arsenide. We can predict the experimental profile over five orders of magnitude for  $\langle 100 \rangle$  and  $\langle 110 \rangle$  channeling and for non-channeling implants at energies up to hundreds of keV.

*Key words:* Molecular Dynamics, Ion Implant, Binary Collision, SIMS, Semiconductors.

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## 1 Introduction

The continuing quest for greater processor performance demands ever smaller device sizes. The effort to realize these ultra shallow junction devices has re-

sulted in current industry trends, such as the use of low energy, high mass, high dose, and large angle implants, to create abrupt dopant profiles. The experimental measurement of such profiles is challenging, as effects that are negligible at high implant energies become increasingly important as the implant energy is lowered. For example, the measurement of dopant profiles by secondary ion mass spectrometry (SIMS) is problematic for very low energy (less than 10 keV) implants, due to limited depth resolution of measured profiles. Also, refining SIMS protocols to obtain profiles for new ion-target combinations, e.g. In, Sb, or N implants or  $\text{Si}_{1-x}\text{Ge}_x$  targets is not a trivial problem.

The use of computer simulation as an alternative method to determine dopant profiles is well established. Binary collision approximation (BCA) codes have traditionally been used, however such simulations become unreliable at low ion energies[1,2]. The BCA approach breaks down when multiple collisions or collisions between moving atoms become significant, or when the crystal binding energy is of the same order as the energy of the ion. Such problems are clearly evident when one attempts to use the BCA to simulate channeling in semiconductors; here the interactions between the ion and target are neither binary nor collisional in nature, rather they occur as many simultaneous soft interactions which steer the ion down the channel.

A more accurate, alternative to the BCA, is the use of molecular dynamics (MD) simulation to calculate ion trajectories[3,4]. However, the computational cost of traditional MD simulations precludes the calculation of the thousands of ion trajectories necessary to construct a dopant profile. Here we present a highly efficient MD-based scheme, that is optimized to calculate the concentration profiles of ions implanted into semiconductors. The algorithms are incorporated into our implant modeling molecular dynamics code[5], REED-MD<sup>1</sup>. Our program has previously been demonstrated to describe the low dose (zero damage) implant of As, B, and P ions with energies in the sub MeV range into crystalline Si in  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and non-channeling directions, and also into amorphous Si[4–6]. We have now extended our model to any ion species, and to other diamond crystal substrates, such as C, Ge, SiC,  $\text{Si}_{1-x}\text{Ge}_x$ , and GaAs. A model for ion induced damage has also been added to the program so that high dose implants can be simulated.

## 2 Molecular Dynamics Model

The basis of the molecular dynamics model is a collection of empirical potential functions that describe interactions between atoms and give rise to forces

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<sup>1</sup> Named for ‘Rare Event Enhanced Domain following Molecular Dynamics’.

between them. In addition to the classical interactions described by the potential functions, the interaction of the ion with the target electrons is required for ion implant simulations, as this is the principle way in which the ion loses energy. Another necessary ingredient is a description of the target material structure, including thermal vibration amplitudes.

Interactions between target atoms are modeled by derivatives of the many-body potential developed by Tersoff[7,8]. ZBL ‘pair specific’ screened Coulomb potentials[9,10] are used to model interactions for common ion-target combinations. For other combinations, the ZBL ‘universal’ potential is used. The ‘universal’ potential is also used to describe the close-range repulsive part of the Tersoff potentials.

We include energy loss due to inelastic collisions, and energy loss due to electronic stopping as two distinct mechanisms. The Firsov model[11] is used to describe the loss of kinetic energy from the ion due to momentum transfer between the electrons of the ion and target atom. We implement this using a velocity dependent pair potential, as derived by Kishinevskii[12].

A modified Brandt-Kitagawa[13] model, that involves both global and local contributions to the electronic stopping is used for electronic energy loss[4,6]. This model contains the single fitted parameter in our scheme,  $r_s^0$ , the ‘average’ one electron radius of the target material experienced by the ion. This is adjusted to account for oscillations in the  $Z_1$  dependence of the electronic stopping cross-section. The parameter is fit once for each ion-target combination and is then valid for all ion energies and incident directions. By using a realistic stopping model, with the minimum of fitted parameters, we obtain a greater transferability to the modeling of implants outside the fitting set.

In the calculations presented here, the target is a {100} diamond crystal with a surface oxide layer. The oxide structure was obtained from annealing a periodic SiO<sub>2</sub> sample with the density constrained to that estimated for grown surface oxide[14]. Thermal vibrations of atoms are modeled by displacing atoms from their lattice sites using a Debye model. For high dose implants, the accumulation of damage within the target is described by a simple Kinchin-Pease[15] model. Target properties are either species dependent, e.g., local electron density, or are obtained by interpolation from known values for single element materials, e.g., lattice constant and Debye temperature.

### 3 Efficient Molecular Dynamics Algorithms

We apply a combination of methods to increase the efficiency of this specific type of simulation. Infrequently updated neighbor lists[16,17] are employed

to minimize the time spent in force calculations. The paths of the atoms are integrated using Verlet’s algorithm[17], with a variable timestep that is dependent upon both kinetic and potential energy of atoms[16].

It is infeasible to calculate dopant profiles by full MD simulation, as computational requirements scale approximately as  $u^4$ , where  $u$  is the initial ion velocity. We have developed a modified MD scheme which is capable of producing accurate dopant profiles with a much smaller computational overhead. We continually create and destroy target atoms, to follow the domain of the substrate that contains the ion. Material is built in front of the ion, and destroyed in its wake. Hence, the ion experiences the equivalent of a complete crystal, but the cost of the algorithm is only  $O(u)$ .

To further improve efficiency, we use three other approximations. The moving atom approximation[3] is used to reduce the number of force calculations. Atoms are divided into two sets; those that are ‘on’ have their positions integrated, and those that are ‘off’ are stationary. At the start of the simulation, only the ion is turned on. Some of the ‘off’ atoms will be used in the force calculations and will have forces assigned to them. If the resultant force exceeds a certain threshold, the atom is turned on. We use two thresholds in our simulation; all atoms interacting directly with the ion are turned on immediately (zero threshold), and other atoms are turned on if the force exceeds  $8.0 \times 10^{-9}$  N.

For high ion velocities, we do not need to use a many-body potential to maintain the stable diamond lattice; a pair potential is sufficient, as only repulsive interactions are significant. Hence, at a certain ion velocity we switch from the complete many-body potential to a pair potential approximation for the target atom interactions. We make a further approximation for still higher ion energies, where only ion-target interactions are significant in determining the ion path. This approximation, termed the recoil interaction approximation[18], brings the MD scheme close to many BCA implementations. The major difference between the two approaches is that the ion path is obtained by integration, rather than by the calculation of asymptotes, and that multiple interactions are, by the nature of the method, handled in the correct manner.

## 4 Rare Event Algorithm

A typical dopant profile in a crystalline semiconductor consists of a near-surface peak followed by an almost exponential decay over several orders of magnitude in concentration. If we attempt to directly calculate a statistically significant dopant concentration at all depths of the profile we will have to run many ions that are stopped near the peak for every one ion that stops in

the tail, and most of the computational effort will not enhance the accuracy of the profile.

In order to remove this redundancy, we employ an ‘atom splitting’ scheme[19] to increase the sampling in the deep component of the concentration profile. At certain splitting depths in the material, each ion is replaced by two ions, each with a statistical weighting of half that prior to splitting. Each split ion trajectory is run separately, and the weighting of the ion is recorded along with its final depth. As the split ions experience different environments (material is built in front of the ion, with random thermal displacements), the trajectories rapidly diverge from one another. Due to this scheme, we can maintain the same number of virtual ions moving at any depth, but their statistical weights decrease with depth. During a typical simulation, 1,000 implanted ions are split to yield around 10,000 virtual ions.

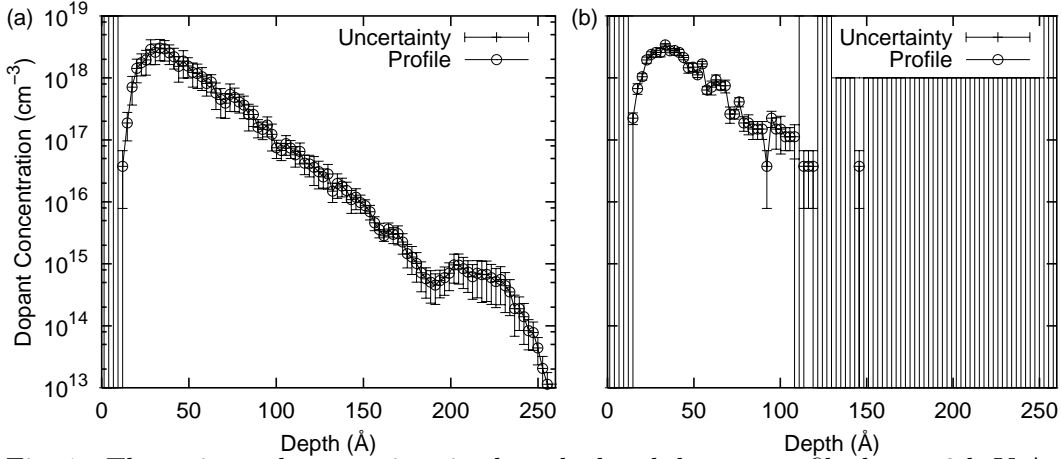


Fig. 1. The estimated uncertainty in the calculated dopant profile due to 2 keV As  $1 \times 10^{12} \text{ cm}^{-2}$  (7,0) implant into Si with 1 unit cell of surface oxide, for the same number of initial ions (1,000), (a) with and (b) without rare event enhancement.

We estimate the uncertainty in the calculated dopant profiles by dividing the final ion depths into 10 sets. A depth profile is calculated from each set using a histogram of 100 bins, and the standard deviation of the distribution of the 10 concentrations for each bin is taken as the uncertainty. Fig. 1 demonstrates the effectiveness of the scheme, by comparing profiles obtained with and without atom splitting over five orders of magnitude. We estimate that the rare event algorithm reduces CPU time by a factor of 90 when calculating profiles over 3 orders of magnitude, and by a factor of 900 when calculating a profile over 5 orders of magnitude.

## 5 Results and Discussion

First, we give 2D profiles for low dose, low energy profiles to show scattering and surface effects. We then give examples of 1D profiles produced by sim-

ulations, and compare to SIMS data[20,21]. All simulations were run with a target temperature of 300 K, and a beam divergence of  $1.0^\circ$  was assumed. Each profile was constructed from 1,000 ions, with the splitting depths updated every 25 ions, and a domain of  $3 \times 3 \times 3$  unit cells was used. The direction of the incident ion beam is specified by the angle of tilt,  $\theta^\circ$ , from normal and the azimuthal angle  $\phi^\circ$ , as  $(\theta, \phi)$ . In the case of the low energy ( $\leq 10$  keV) implants, we assume one unit cell thickness of surface oxide; for other cases we assume three unit cells of oxide at the surface. For the low energy implants, we have calculated profiles over a change of five orders of magnitude in concentration; for the higher energy implants we calculate profiles over 3 orders of magnitude. A dose of  $1 \times 10^{12} \text{ cm}^{-2}$  (zero damage) is used unless otherwise noted.

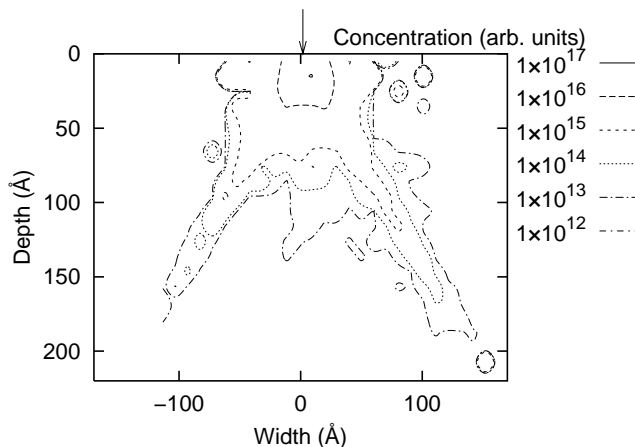


Fig. 2. Calculated 2D dopant profile due to 0.2 keV B (0,0) implant into Si.

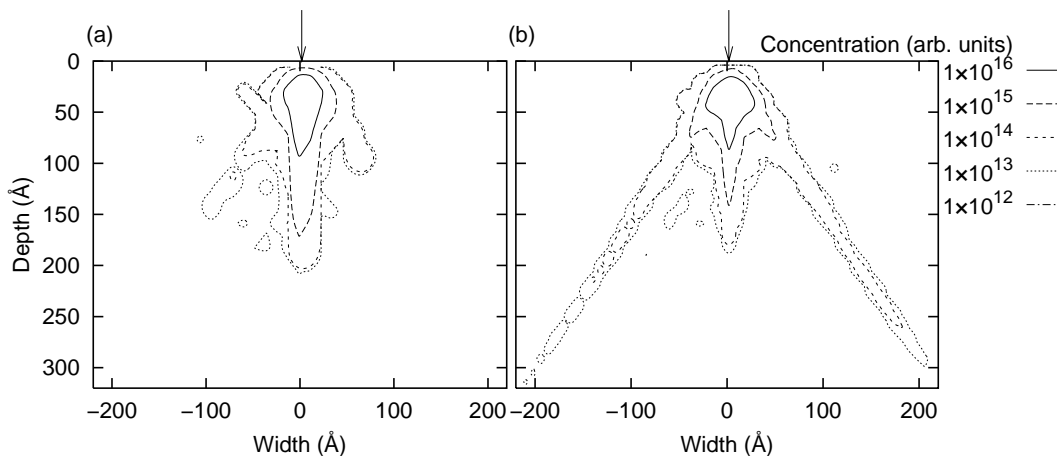


Fig. 3. Calculated 2D dopant profiles due to 2 keV As (0,0) implants into Si, with (a) 1 and (b) 3 unit cells of surface oxide.

2D profiles are shown projected onto the plane normal to the surface and containing the zero degree azimuth. This makes it easy to differentiate between major channeling directions; the  $\langle 100 \rangle$  channel is vertical, and the four  $\langle 110 \rangle$  channels appear at angles of  $35^\circ$  from vertical. Fig. 2 shows the result of an ultra-low energy implant into Si. Although the implant is in the  $\langle 100 \rangle$  direction, this channel is closed at such low ion energies and the only channeling

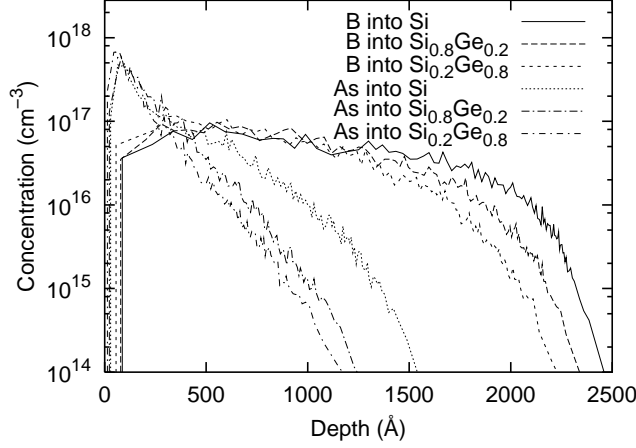


Fig. 4. Calculated dopant profiles for 10 keV B and As (0,0) implants into  $\text{Si}_{1-x}\text{Ge}_x$ .

occurs in the  $\langle 110 \rangle$  direction. This demonstrates the need to have a ‘universal’ electronic stopping model, rather than a model tuned for a particular channeling direction. The effect of the amount of surface disorder is shown in Fig. 3. Increasing the thickness of the surface layer leads to more ions being scattered into the larger  $\langle 110 \rangle$  channel, and hence gives a far deeper tail to the profile.

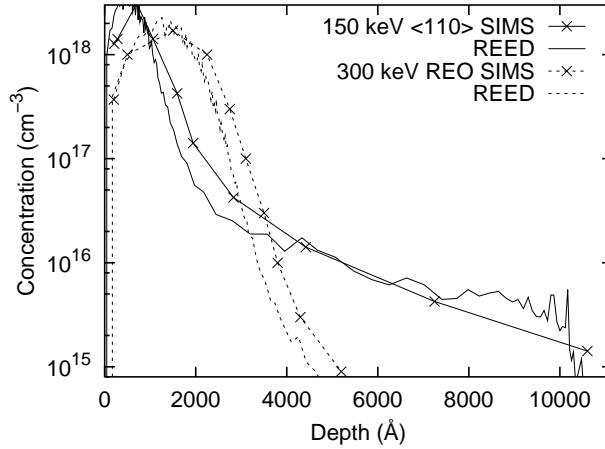


Fig. 5. Calculated and experimental[20] dopant profiles due to  $\text{Zn } 3 \times 10^{13} \text{ cm}^{-2}$  implants into GaAs.

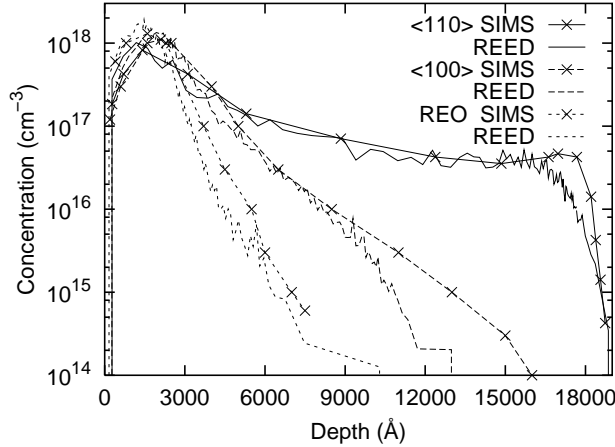


Fig. 6. The calculated and experimental[21] dopant profiles due to 150 keV  $\text{Si } 3 \times 10^{13} \text{ cm}^{-2}$  implants into GaAs.

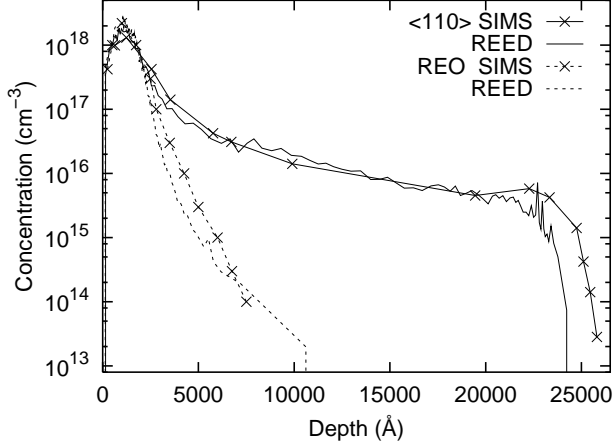


Fig. 7. The calculated and experimental[21] dopant profiles due to 300 keV Se  $3 \times 10^{13} \text{ cm}^{-2}$  implants into GaAs.

There is increasing interest in the use of SiGe as a replacement for Si currently used in CMOS technology, due to its higher switching speed[22]. Fig. 4 shows the effect of Ge concentration on profiles from B and As implants into  $\text{Si}_{1-x}\text{Ge}_x$  targets. The trend is clearly for shallower profiles with increasing Ge concentration, but this is extremely non-linear; the difference between  $x = 0$  and  $x = 0.2$  profiles is greater than the difference between  $x = 0.2$  and  $x = 0.8$  profiles. The remaining figures show the calculated concentration profiles of several ion species implanted under various conditions into GaAs substrates, and comparison with available SIMS data. The results of the REED calculations show good agreement with the experimental data, demonstrating the accuracy of our model and its transferability to many ion-target combinations and implant conditions.

## 6 Conclusions

In summary, we have developed a restricted MD code to simulate the ion implant process and calculate ‘as implanted’ dopant profiles. This gives us the accuracy obtained by time integrating atom paths, with an efficiency far in excess of full MD simulation.

The scheme described here gives a viable alternative to the BCA approach. Although it is still more expensive computationally, it is sufficiently fast to be used on modern desktop computer workstations. The method has two major advantages over the BCA approach: (i) Our MD model consists only of standard empirical potentials developed for bulk semiconductors and for ion-solid interactions. The only fitting is in the electronic stopping model, and this involves *only one* parameter per ion-target combination. We believe that by using physically based models for all aspects of the program, with the minimum of fitting parameters, we obtain good transferability to the mod-



eling of implants outside of our fitting set. (ii) The method does not break down at the low ion energies necessary for production of the next generation of semiconductor technology; it gives the correct description of multiple, soft interactions that occur both in low energy implants, and higher energy channeling. Hence our method remains truly predictive at these low ion energies, whilst the accuracy of the BCA is in doubt.

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